

Adjoint sensitivity analysis of radiative transfer equation: temperature and gas mixing ratio weighting functions for remote sensing of scattering atmospheres in thermal IR

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Abstract

Sensitivity analysis based on using of the adjoint equation of radiative transfer is applied to the case of atmospheric remote sensing in the thermal spectral region with non-negligible atmospheric scattering. Analytic expressions for the weighting functions for retrievals of temperature and gas mixing ratio are derived. It is demonstrated that these expressions include the case of pure absorption as a particular case when single scattering albedo of atmospheric scattering can be neglected.

1 Introduction

Various geophysical applications involve modeling of radiative fluxes in the atmosphere or simulation of observable data for given atmospheric models. This task is accomplished by solving the differential equation of radiative transfer with corresponding boundary conditions. The modeled radiative quantities depend on vertical profiles of atmospheric parameters and sensitivity of them to these profiles is also an important subject of study. The inversion of observations in terms of vertical profiles of the atmospheric parameters poses a similar problem. The needs of development of new instruments for remote sensing also require predictions how sensitive are measured data to atmospheric profiles such as temperature or mixing ratio of gaseous constituents.

The sensitivities of radiative quantities J to atmospheric parameters X can be quantitatively described by the variational derivatives $\delta J/\delta X$. If, e.g., we observe the radiances at the top of atmosphere $J_\nu(\Omega)$ for a set of frequencies ν and/or directions Ω and intend to retrieve the vertical profile of an

atmospheric parameter $X(\zeta)$ with respect to some coordinate, ζ , we assume herewith that there exists an, in general, non-linear operator dependence between the radiance $J_\nu(\Omega)$ and $X(\zeta)$. The variations, δJ and δX , are related through linear integral equation

$$\delta J_\nu(\Omega) = \int_Z K_\nu^{(X)}(\zeta, \Omega) \delta X(\zeta) d\zeta. \quad (1)$$

The kernel in the integral term of this equation, $K_\nu^{(X)}(\zeta, \Omega)$, labeled by parameter X ,

$$K_\nu^{(X)}(\zeta, \Omega) = \frac{\delta J_\nu(\Omega)}{\delta X(\zeta)} \quad (2)$$

is the corresponding variational derivative for this case. It also has a meaning of a weighting function for the parameter $X(\zeta)$, which determines the input of variation $\delta X(\zeta)$ into $\delta J(\Omega)$. Also, Eq.2 gives a measure of sensitivity of J to X . With weighing functions $K_\nu^{(X)}(\zeta, \Omega)$ computed for a set of selected ν and/or Ω for some initial atmospheric model, a corresponding linearized inverse problem can be considered in the form of a corresponding linear integral equation (cf. Eq.1):

$$\int_Z K_\nu^{(X)}(\zeta, \Omega) \Delta X(\zeta) d\zeta = \Delta J_\nu(\Omega). \quad (3)$$

If radiative quantities J can be directly expressed analytically through atmospheric parameters X then their sensitivities to these parameters, $\delta J/\delta X$ can also be evaluated analytically. A well-known example is given by remote sensing of a purely absorbing atmosphere in thermal spectral region. There is no dependence on azimuth angle and, for nadir viewing geometry, the direction of the line of sight can be specified by its zenith angle, $\cos^{-1}\mu$. Log pressure, $\ln p$, can be used as a vertical coordinate. The temperature weighting functions at given ν and μ ,

$$K_\nu^{(T)}(p, \mu) = \frac{\delta J_\nu(\mu)}{\delta T(p)} = -\frac{\partial t_\nu}{\partial \ln p} \cdot \frac{dB_\nu}{dT} \Big|_{T(p)}, \quad (4)$$

are analytically expressed the atmospheric transmittance functions at frequencies ν , $t_\nu(p, \mu)$ and Planck function, $B_\nu(T)$ which can be evaluated for given models of temperature and atmospheric opacity. Similarly, the gas mixing ratio weighting functions for retrieval of the gaseous atmospheric constituents,

$$K_\nu^{(f)}(p, \mu) = \frac{\delta J_\nu(\mu)}{\delta \ln f(p)} = -\frac{1}{\mu} H_g(p) \kappa_\nu(p) \int_p^{p_0} t_\nu(p, \mu) dB_\nu(T(p)), \quad (5)$$

are also analytically expressed through $t_\nu(p, \mu)$, $B_\nu(T)$ and volume absorption coefficient, κ_ν of the constituent. H_g is the scale height of gaseous atmosphere [1], [2].

If the atmospheric scattering is non-negligible then analytic expressions for modeled/simulated radiative quantities are not available. There exist a wide variety of numerical methods for solution of the differential equation of radiative transfer that make it possible to compute radiative quantities for any plausible atmospheric models. As for the weighting functions of corresponding inverse problems, the way most widely used so far is to divide the atmosphere into computationally affordable number of layers, to vary the profiles of atmospheric parameters involved, layer by layer, to obtain corresponding solutions of the equation of radiative transfer and finally to evaluate the responses of radiative quantities to these variations. Obviously, this method requires much greater expenditures of computing time as compared to the single run needed to model radiances themselves.

There exists an alternative approach that was introduced into the field of atmospheric remote sensing by Marchuk [3] more than three decades ago. In general, if a linear or linearized forward equation is used to model an object under study, then a *single* solution of the corresponding adjoint equation can be used to compute the sensitivities to all parameters of the model. The adjoint equation is similar to its forward counterpart and both can be solved by the same methods. Use of this approach dramatically reduces the computing time needed to compute the resulting sensitivities.

The applications of the adjoint approach to sensitivity analysis in remote sensing area started about a decade ago. Box et al. [4] have introduced the adjoint equation of radiative transfer (independently of Marchuk [3]) and discussed possible applications of it in the sensitivity analysis. Sensitivities of scattered solar radiation fluxes and heating rates to perturbations of aerosol in cloudless atmospheres were studied in [5] and [6]. We applied this approach to analytic studies of the case of thermal radiation in the purely absorbing atmosphere [1] and of the case of solar radiation reflected from the scattering, optically thick vertically inhomogeneous planetary atmosphere [8], [9], [10]. Box and Sendra [11] studied the sensitivity of emergent radiation to the shape of the phase function for vertically homogeneous atmospheres with the intention of using these results in the remote sensing in the solar spectral region. In their recent publications, [12], [13] (see also references therein) the practical retrieval issues were studied.

Here we consider the applications of adjoint sensitivity analysis to retrievals of temperature and gas mixing ratio from remote sensing data in the thermal IR. We will address the formulation of the adjoint RT problem in a way that explicitly produces its components, the adjoint RT equation and its upper and

lower boundary conditions corresponding to their counterparts in the forward problem of radiative transfer.

We first consider the general operator formulation [3] resulting in an explicit expression for the variational derivatives. This expression is further applied to the analysis of sensitivity of observed radiances to vertical profiles of temperature and gas mixing ratio. Expressions for corresponding temperature and mixing ratio weighting functions will be derived. As it will be demonstrated, these expressions include the temperature and mixing ratio weighting functions for the case of pure absorption, [1], [2] as a particular case if the atmospheric scattering can be neglected.

2 General operator formulation of the adjoint approach

In this Section we present the general methodology developed by Marchuk [3]. The forward problem of radiative transfer in the thermal IR for a plane-parallel atmosphere can be written in the form:

$$u \frac{dI}{d\tau} + I(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u, u') I(\tau, u') du' = (1 - \omega_0(\tau)) B(T(\tau)), \quad (6)$$

$$I(0, u) = 0, \quad u > 0, \quad (7)$$

$$I(\tau_0, u) - 2A \int_0^1 I(\tau_0, u') u' du' = (1 - A) B(T_0). \quad u < 0. \quad (8)$$

Here $I(\tau, u)$ is the intensity of radiation which depends on the optical depth τ measured from the upper boundary of the atmosphere and on the nadir angle, $\cos^{-1} u$, measured from the nadir direction; $p(\tau; u, u')$ is the phase function of atmospheric scattering; $\omega_0(\tau)$ is a single scattering albedo; $B(T)$ is blackbody radiance at temperature T ; A and $B(T_0)$ are Lambertian albedo and thermal radiance of the surface at temperature T_0 . Because the source thermal radiation is isotropic, there is no dependence on the azimuth angle. The frequency, ν , is implied.

The observable radiative quantities, J are related to the total field of I in the form of convolution with some function, W describing both the instrument and geometry of observations. The measured radiances can be presented in the form of convolution:

$$J(\mu) = \int_0^{\tau_0} \int_{-1}^1 W(\mu; \tau, u) I(\tau, u) du d\tau. \quad (9)$$

E.g., for the instrument with infinitesimally small field of view placed outside the atmosphere,

$$W(\mu; \tau, u) = \delta(\tau)\delta(u + \mu). \quad (10)$$

Both W and I are functions of τ and u and are defined in the same domain. Their convolution, Eq.9, can be considered as a scalar product of these functions:

$$J = (W, I). \quad (11)$$

Let the forward problem of radiative transfer, Eqs.6–8, can be represented in the form of a linear operator equation

$$L I = S, \quad (12)$$

where the linear operator L combines all operations with intensity I in left-hand terms of Eqs.6–8 and function S combines the inhomogeneous terms in the right-hand terms. Below we will use the abbreviated notations like Eqs.11, 12 that make the derivations more compact. The general way to construct attributes L and S of the forward RT problem and to derive corresponding attributes, L^* and W of the adjoint RT problem will be developed in the next Section. By definition, for a given linear operator L , the adjoint operator L^* satisfies the identity

$$(L f, g) = (f, L^* g), \quad (13)$$

where f and g are two arbitrary functions from the domain of L . Let function $I^*(\tau, u)$ be solution of the linear operator equation

$$L^* I^* = W, \quad (14)$$

where L^* is an operator, adjoint to L and the right-side term W in the right hand contains the function W defining the observed radiances, J , in the form of Eq.11. It should be noted that in this way, the term W of the adjoint problem Eq.14 and its solution I^* contains the dependence on geometry of observations described here by the parameter μ .

The first important result of application of the adjoint approach is that the adjoint solution I^* provides a way, alternative to Eq.11 to compute the observable quantities, J :

$$J = (I^*, S). \quad (15)$$

Indeed, multiplying Eq.12, by I^* and Eq.14 by I we have:

$$(I^*, LI) = (I^*, S), \quad (16)$$

$$(L^*I^*, I) = (W, I). \quad (17)$$

The left sides of Eqs.16, 17 are equal by definition, Eq.13. Replacing the right hand of Eq.17 by J according to Eq.11 we immediately obtain Eq.15.

The second, even more important result of application of the adjoint approach is that the adjoint solution I^* together with the forward solution I provides an easily computable expression for the variational derivatives *alias* weighting functions $\delta J/\delta X$. Let $J(\mu)$ be the radiative quantities computed by Eq.6 from the solution I of the forward problem, Eq.7, for an atmospheric model specified by a set of vertical profiles of n atmospheric parameters X_i ($i = 1, \dots, n$). Let J' be the radiative quantities computed from the solution I' of the perturbed forward problem,

$$L'I' = S' \quad (18)$$

for an atmospheric model specified by a set of perturbed parameters $X'_i = X_i + \delta X_i$ resulting into perturbed operator, L' , and right hand term, S' . Subtracting Eq.12 from Eq.18 and keeping only the linear variations we have:

$$L\delta I + \delta LI = \delta S. \quad (19)$$

Multiplying both sides of Eq.19 by I^* we obtain:

$$(L\delta I, I^*) + (\delta LI, I^*) = (\delta S, I^*). \quad (20)$$

On the other hand, multiplying both sides of the adjoint problem, Eq.14, by the variation of solution of the forward problem, δI , we have:

$$(\delta I, L^*I^*) = (\delta I, W). \quad (21)$$

From the definition of J , Eq.11, the right-hand term of Eq.21 is equal to its variation, δJ . Replacing this term by δJ , substituting the result into Eq.20 and using the definition of L^* , Eq.13 applied to functions δI and I^* we obtain the expression for variation δJ through solutions I , I^* and variations δL and δS :

$$\delta J = (\delta S - \delta LI, I^*). \quad (22)$$

The variations of δS , δL , and δJ can be expressed through variations of atmospheric parameters, δX_i using corresponding variational derivatives:

$$\delta L = \sum_i \int \frac{\delta L}{\delta X_i} \delta X_i d\zeta, \quad \delta S = \sum_i \int \frac{\delta S}{\delta X_i} \delta X_i d\zeta, \quad (23)$$

$$\delta J = \sum_i \int \frac{\delta J}{\delta X_i} \delta X_i d\zeta. \quad (24)$$

Thus, the equation for these variations can be rewritten in the form:

$$\sum_i \frac{\delta J}{\delta X_i} \delta X_i = \sum_i \left(\frac{\delta S}{\delta X_i} - \frac{\delta L}{\delta X_i} I, I^* \right) \delta X_i, \quad (25)$$

Requiring that Eqs.23–25 for arbitrary variations δX_i , we obtain:

$$\frac{\delta J}{\delta X_i} = \left(\frac{\delta S}{\delta X_i} - \frac{\delta L}{\delta X_i} I, I^* \right). \quad (26)$$

The expression Eq.26 provides the way of computing the weighting functions for any parameters that enter the forward problem of radiative transfer through its operator L and the right-term S . Below, this expression is used to obtain the temperature and gas mixing ratio weighting functions.

3 Formulation of the adjoint problem of radiative transfer in a scattering atmosphere in thermal IR

We first rewrite the forward problem of radiative transfer, Eq.6–8 in a general form:

$$L_e I - S_e = 0 \quad (27)$$

$$L_t I - S_t = 0, \quad \tau = 0, \quad u > 0 \quad (28)$$

$$L_b I - S_b = 0, \quad \tau = \tau_0, \quad u < 0 \quad (29)$$

where the subscripts 'e', 't' and 'b' stand for 'equation', upper ('top') and lower ('bottom') boundary conditions respectively. Operators L_e , L_t and L_b have the form:

$$L_e I = u \frac{dI}{d\tau} + I(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u, u') I(\tau, u') du', \quad (30)$$

$$L_t I = I(0, u), \quad (31)$$

$$L_b = I(\tau_0, u) - 2A \int_0^1 I(\tau_0, u') u' du'. \quad (32)$$

Operator L_e is describing the linear operations on I in the whole domain of arguments $\tau \in [0, \tau_0]$ and $u \in [-1, 1]$. Unlike operator L_e , operators L_t and L_b are limited in action with respect to both τ and u . The operator L_t is essentially the identity operator but its action is limited to the upper boundary $\tau = 0$ and upper hemisphere, $u > 0$. Similarly, the action of the operator L_b is limited to the lower boundary, $\tau = \tau_0$ and lower hemisphere, $u < 0$. To enforce these restrictions, we use appropriate weighting factors containing Dirac δ -functions over τ and Heavyside θ -functions over u :

$$\delta(\tau)\theta(u)(L_t I - S_t) = 0 \quad (33)$$

$$\delta(\tau_0 - \tau)\theta(-u)(L_b I - S_b) = 0 \quad (34)$$

It should be noted that Eqs.33, 34 remain equivalent to the boundary conditions, Eqs.31, 32 if they are multiplied by arbitrary functions of τ and/or u that are non-zero everywhere where the above weighting factors are non-zero. For reasons that will be clear below (see a remark after Eq.45), we multiply Eqs.33, 34 by u and $-u$ respectively:

$$\delta(\tau)u\theta(u)(L_t I - S_t) = 0 \quad (35)$$

$$\delta(\tau_0 - \tau)(-u)\theta(-u)(L_b I - S_b) = 0 \quad (36)$$

Adding Eqs.27, 35, 36 and moving terms with S_e , S_t , and S_b into the right side of the resulting linear operator equation, we obtain

$$(L_e + \delta(\tau)u\theta(u)L_t - \delta(\tau_0 - \tau)u\theta(-u)L_b)I = S_e + \delta(\tau)u\theta(u)S_t - \delta(\tau_0 - \tau)u\theta(-u)S_b \quad (37)$$

Introducing the function $\lambda(u)$ by definition

$$\lambda(u) = u\theta(u) \quad \left(\frac{d\lambda}{du} = \theta(u) \right) \quad (38)$$

we obtain:

$$(L_e + \delta(\tau)\lambda(u)L_t + \delta(\tau_0 - \tau)\lambda(-u)L_b)I = S_e + \delta(\tau)\lambda(u)S_t + \delta(\tau_0 - \tau)\lambda(-u)S_b \quad (39)$$

Equation 39 has the form of a single scalar linear operator equation Eq.12 where the linear operator L contains all operations on I in the forward RT problem, Eqs.6, 7, 8 or Eqs.30, 31, 32 respectively:

$$L I = L_e I + \delta(\tau)\lambda(u)L_t I + \delta(\tau_0 - \tau)\lambda(-u)L_b I. \quad (40)$$

In the remainder of this Section we derive the operator L^* , adjoint to the operator L defined by Eqs.40, 30–32 using the formal definition, Eq.13 applied to arbitrary functions $I(\tau, u)$ and $I^*(\tau, u)$ from the domain of the operator L :

$$(L I, I^*) = (I, L^* I^*) \quad (41)$$

3.1 Case for the lower boundary condition with $A = 0$

We first consider the simpler case of the lower boundary condition, Eq.8, corresponding to $A = 0$. Substituting Eq.40 into Eq.41 and using the definition of function $\lambda(u)$, Eq.38 we have:

$$\begin{aligned} (L I, I^*) &= \\ &= \int_{-1}^1 du \left\{ \int_0^{\tau_0} d\tau \left[u \frac{dI}{d\tau} + I(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u, u') I(\tau, u') du' \right] I^*(\tau, u) + \right. \\ &\quad \left. + \lambda(u) I(0, u) I^*(0, u) + \lambda(-u) I(\tau_0, u) I^*(\tau_0, u) \right\}. \end{aligned} \quad (42)$$

For the first and third terms in square parentheses we have:

$$\begin{aligned} &\int_{-1}^1 du \int_0^{\tau_0} d\tau u \frac{dI}{d\tau} I^*(\tau, u) = \\ &= \int_{-1}^1 du \left[u I(\tau_0, u) I^*(\tau_0, u) - u I(0, u) I^*(0, u) + \right. \\ &\quad \left. + \int_0^{\tau_0} d\tau I(\tau, u) \left(-u \frac{dI^*}{d\tau} \right) \right]; \end{aligned} \quad (43)$$

The integral in square parentheses can be written in the form:

$$\begin{aligned}
& \int_{-1}^1 du \int_0^{\tau_0} d\tau \left[\int_{-1}^1 p(\tau; u, u') I(\tau, u') du' \right] I^*(\tau, u) = \\
& = \int_{-1}^1 du \int_0^{\tau_0} d\tau I(\tau, u) \left[\int_{-1}^1 p(\tau; u', u) I^*(\tau, u') du' \right]. \tag{44}
\end{aligned}$$

After substitution into Eq.42, combining terms at $\tau = 0$ and $\tau = \tau_0$ we have:

$$\begin{aligned}
& (L I, I^*) = \\
& = \int_{-1}^1 du \left\{ \int_0^{\tau_0} d\tau I(\tau, u) \left[-u \frac{dI^*}{d\tau} + I^*(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u', u) I^*(\tau, u') du' \right] - \right. \\
& \quad \left. -u[1 - \theta(u)]I(0, u)I^*(0, u) + u[1 - \theta(-u)]I(\tau_0, u)I^*(\tau_0, u) \right\} \tag{45}
\end{aligned}$$

We have used a freedom of choice stated above and multiplied Eqs.33, 34 by u and $-u$ respectively, to be able to combine the terms at $\tau = 0$ and $\tau = \tau_0$ in Eq.45. Using the identity

$$\theta(-u) + \theta(u) = 1, \tag{46}$$

we can rewrite Eq.45 in the form:

$$\begin{aligned}
& (L I, I^*) = \\
& = \int_{-1}^1 du \left\{ \int_0^{\tau_0} d\tau I(\tau, u) \left[-u \frac{dI^*}{d\tau} + I^*(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u', u) I^*(\tau, u') du' \right] + \right. \\
& \quad \left. + \lambda(-u)I(0, u)I^*(0, u) + \lambda(u)I(\tau_0, u)I^*(\tau_0, u) \right\} \tag{47}
\end{aligned}$$

Equation 21 may be written in the desired form of scalar product, $(I, L^* I^*)$, in the right side of definition, Eq.15. Using the definition of function $\lambda(u)$, Eq.11, we have:

$$L^* I^* = L_e^* I^* + \delta(\tau) \lambda(-u) L_t^* I^* + \delta(\tau_0 - \tau) \lambda(u) L_b^* I^*. \tag{48}$$

Here, the operator L_e^* is describing the linear operations on I^* in the whole domain of $\tau \in [0, \tau_0]$ and $u \in [-1, 1]$:

$$L_e^* I^* = -u \frac{dI^*}{d\tau} + I^*(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u', u) I^*(\tau, u') du' \tag{49}$$

and, as δ -functions in Eq.48 imply, operator L_t^* acts at the upper boundary, $\tau = 0$ and operator L_b^* acts at the lower boundary, $\tau = \tau_0$. Also, the θ -functions limit action of operators L_t^* and L_b^* to the lower and upper hemispheres respectively. With these limitations specified we have:

$$L_t^* I^* = I^*(0, u), \quad u < 0, \quad (50)$$

$$L_b^* I^* = I^*(\tau_0, u), \quad u > 0, \quad (51)$$

Operator L^* , Eq.48 satisfies the definition, Eqs.13, 41 and is herewith an operator adjoint to the operator of the forward RT problem, Eqs.6–8. Its component, L_b^b defined by Eq.51 corresponds to the simplified lower boundary condition of the forward RT problem, Eq.8, with $A = 0$.

Denoting the right side terms of the equation of the adjoint RT problem and of its boundary conditions as, respectively, W_e , W_t , and W_b we can write the resulting adjoint problem of radiative transfer in the following form:

$$-u \frac{dI^*}{d\tau} + I^*(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u', u) I^*(\tau, u') du' = W_e(\tau, u), \quad (52)$$

$$I^*(0, u) = W_t(u), \quad u < 0, \quad (53)$$

$$I^*(\tau_0, u) = W_b(u), \quad u > 0. \quad (54)$$

3.2 General case for the lower boundary condition with $A \neq 0$

Substituting Eq.40 into Eq.41 and using the definition for $\lambda(u)$, Eq.38, we have:

$$\begin{aligned} (L I, I^*) = & \int_{-1}^1 du \left\{ \int_0^{\tau_0} d\tau \left[u \frac{dI}{d\tau} + I(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u, u') I(\tau, u') du' \right] I^*(\tau, u) + \right. \\ & \lambda(u) I(0, u) I^*(0, u) + \\ & \left. \lambda(-u) \left[I(\tau_0, u) - 2A \int_0^1 I(\tau_0, u') u' du' \right] I^*(\tau_0, u) \right\}. \end{aligned} \quad (55)$$

Comparing Eq.55 with Eq.42 we see that it contains an extra term due to

$A \neq 0$:

$$\Delta_A(L I, I^*) = - \int_{-1}^1 du \lambda(-u) \left[2A \int_0^1 I(\tau_0, u') u' du' \right] I^*(\tau_0, u) \quad (56)$$

which can be rewritten in the form (cf. Eq.38):

$$\Delta_A(L I, I^*) = \int_{-1}^1 du u \theta(u) I(\tau_0, u) \cdot 2A \int_{-1}^0 I^*(\tau_0, u') u' du' \quad (57)$$

After substitution of Eq.57 together with Eqs.43, 44 into Eq.55, combining terms at $\tau = 0$, $\tau = \tau_0$ and using the identity, Eq.46 we obtain:

$$\begin{aligned} (L I, I^*) = & \int_{-1}^1 du \left\{ \int_0^{\tau_0} d\tau I(\tau, u) \left[-u \frac{dI^*}{d\tau} + I^*(\tau, u) - \frac{1}{2} \int_{-1}^1 p(\tau; u', u) I^*(\tau, u') du' \right] - \right. \\ & u \theta(-u) I(0, u) I^*(0, u) + \\ & \left. u \theta(u) I(\tau_0, u) \left[I^*(\tau_0, u) + 2A \int_{-1}^0 I^*(\tau_0, u') u' du' \right] \right\} \end{aligned} \quad (58)$$

The right side of Eq.58 can be written in the form of scalar product, $(I, L^* I^*)$ in the right side of definition, Eq.41, if we let the adjoint operator to be defined by Eq.48, with components, L_e^* and L_i^* defined by Eqs.49, 50 but with L_b^* now defined in the form:

$$L_b^* I^* = I^*(\tau_0, u) + 2A \int_{-1}^0 I^*(\tau_0, u') u' du', \quad u > 0. \quad (59)$$

Thus, the resulting lower boundary condition of the adjoint problem considered here has the form:

$$I^*(\tau_0, u) + 2A \int_{-1}^0 I^*(\tau_0, u') u' du' = W_b(u), \quad u > 0. \quad (60)$$

3.3 Formulation of the adjoint problem of radiative transfer: A summary

The forward RT problem

$$\begin{aligned}
L_e I &= S_e \\
L_t I &= S_t, \quad u > 0 \\
L_b I &= S_b, \quad u < 0
\end{aligned} \tag{61}$$

is represented in the form of a single linear operator equation $L I = S$ by using weighting factors

$$\begin{aligned}
w_e(\tau, u) &= 1 \\
w_t(\tau, u) &= \delta(\tau) \lambda(u) \\
w_b(\tau, u) &= \delta(\tau_0 - \tau) \lambda(-u)
\end{aligned} \tag{62}$$

which specify the range over τ and u where each component of the system, Eq.61 is valid. Using a symbolic index i , ($i = e, t, b$):

$$L = \sum_i w_i L_i \tag{63}$$

$$S = \sum_i w_i S_i \tag{64}$$

The linear operator of corresponding adjoint RT problem in the operator form, $L^* I = W$ is obtained directly by applying the definition, Eq.41, with arbitrary I and I^* . The scalar product (I^*, LI) is further transformed to the form $(L^* I^*, I)$ and the operator L^* , adjoint to L , is obtained in the form:

$$L^* = \sum_i w_i^* L_i^* \tag{65}$$

with weighting factors w_i^* :

$$\begin{aligned}
w_e^*(\tau, u) &= 1 \\
w_t^*(\tau, u) &= \delta(\tau) \lambda(-u) \\
w_b^*(\tau, u) &= \delta(\tau_0 - \tau) \lambda(u)
\end{aligned} \tag{66}$$

The form of each linear operator L_i^* is defined by the specific form of corresponding operator L_i . The right-hand term of the corresponding adjoint problem of radiative transfer W is represented as a sum:

$$W = \sum_i w_i^* W_i \tag{67}$$

Its separate components, W_e , W_t , and W_b can be obtained by representing the expression for the observed radiances, J , in the form

$$J = \sum_i w_i^*(W_i, I) \quad (68)$$

4 Temperature and gas mixing ratio weighting functions

In this Section we will demonstrate how the variational relation, Eq.2.17 is used for evaluation of sensitivities of observed radiances to atmospheric parameters. The concrete atmospheric parameters that will be considered here are temperature T and volume mixing ratio f of the absorbing atmospheric constituent.

4.1 Temperature weighting functions

We first obtain the temperature weighing functions, $\delta J/\delta T$ that will provide a generalization of the case of pure absorption, Eq.4, to the case with atmospheric scattering. Here we assume that only temperature, δT is varied. Then $\delta L \equiv 0$ and the expression for δJ , Eq.22 takes the form:

$$\delta J = (\delta S, I^*). \quad (69)$$

Substituting the variation of right-hand term of Eq.6,

$$\delta S(\tau, u) = (1 - \omega_0(\tau)) \frac{dB}{dT} \Big|_{T(\tau)} \delta T(\tau), \quad (70)$$

into Eq.69, using the explicit form of the scalar product, and rearranging the multiplicands we have:

$$\delta J(\mu) = \int_0^{\tau_0} d\tau \delta T(\tau) (1 - \omega_0(\tau)) \frac{dB}{dT} \Big|_{T(\tau)} \int_{-1}^1 du I^*(\tau, u). \quad (71)$$

Comparing Eq.72 with Eq.1 we obtain the expression for temperature weighing functions in the form:

$$\frac{\delta J(\mu)}{\delta T(\tau)} = (1 - \omega_0(\tau)) \frac{dB}{dT} \Big|_{T(\tau)} \int_{-1}^1 I^*(\tau, u) du. \quad (72)$$

This is a sought generalization of the case of pure absorption, Eq.4. To demonstrate that Eq.72 is indeed a particular case of Eq.4 we consider the adjoint problem of radiative transfer, Eq.55, 56, 57, for the case of pure absorption ($\omega_0 = 0$) with a right-hand term defined by Eq.10:

$$-u \frac{dI^*}{d\tau} + I^*(\tau, u) = \delta(\tau) \delta(u + \mu), \quad (73)$$

$$I^*(0, u) = 0, \quad u < 0, \quad (74)$$

$$I^*(\tau_0, u) = 0, \quad u > 0. \quad (75)$$

Its solution for the upwelling radiation ($u = -\mu$) is [1]:

$$I^*(\tau, u) = \frac{1}{\mu} \exp(-\tau/\mu) \delta(u + \mu), \quad (76)$$

and Eq.72 takes the form:

$$\frac{\delta J(\mu)}{\delta T(\tau)} = \frac{dB}{dT} \Big|_{T(\tau)} \cdot \frac{1}{\mu} \exp(-\tau/\mu). \quad (77)$$

Introducing atmospheric transmittance, $t(\tau, \mu)$

$$t(\tau, \mu) = \exp(-\tau/\mu), \quad (78)$$

$$\frac{\partial t}{\partial \tau} = -\frac{1}{\mu} \exp(-\tau/\mu), \quad (79)$$

we can rewrite Eq.77 in the form:

$$\frac{\delta J(\mu)}{\delta T(\tau)} = -\frac{\partial t}{\partial \tau} \cdot \frac{dB}{dT} \Big|_{T(\tau)}. \quad (80)$$

Finally, changing the vertical coordinate from τ to p and using $\ln p$ for the differentiation in Eq.10 and subsequent integration, we have to multiply Eq.10 by factor $d\tau/d \ln p$. This results in the expression for pure absorption in the form of Eq.4.

4.2 Volume mixing ratio weighting functions

The case for the gas mixing ratio weighing functions, $\delta J/\delta f$ needs more analytic work because both L and S experience variations if the gas mixing ratio

f is varied. To single out the dependence of L and S on f we first consider the general case of an atmosphere consisting of two components: an known background atmosphere described by the optical depth τ and phase function $p(\tau, u)$ and unknown constituent producing an additional optical depth, $\tau^{(1)}(\tau)$ and, in general, additional atmospheric scattering described by phase function $p^{(1)}(\tau, u)$ [10]. For the composite optical depth, $\tau^{(\Sigma)}(\tau)$, and phase function, $p^{(\Sigma)}(\tau, u)$ of such two-component atmosphere we have:

$$d\tau^{(\Sigma)} = d\tau + d\tau^{(1)}, \quad (81)$$

$$p^{(\Sigma)} d\tau^{(\Sigma)} = p d\tau + p^{(1)} d\tau^{(1)}. \quad (82)$$

In particular, for the purely absorbing gas, $p^{(1)} \equiv 0$ and we have:

$$p^{(\Sigma)} d\tau^{(\Sigma)} = p d\tau. \quad (83)$$

We further introduce the *optical* mixing ratio of the unknown component, $f^{(1)}$, defined by ratio

$$f^{(1)}(\tau) = \frac{d\tau^{(1)}}{d\tau}. \quad (84)$$

Then Eqs.81 and 82 can be rewritten in the form:

$$d\tau^{(\Sigma)} = (1 + f^{(1)}) d\tau, \quad (85)$$

$$(1 + f^{(1)})p^{(\Sigma)} = (p + f^{(1)}p^{(1)}). \quad (86)$$

In particular, from Eq.86 it follows that for the single scattering albedo, ω_0 , we have:

$$(1 + f^{(1)})\omega_0^{(\Sigma)} = \omega_0 + f^{(1)}\omega_0^{(1)}. \quad (87)$$

and for the emissivity factor, $1 - \omega_0$ in the right-hand term S of Eq.6 we have:

$$(1 + f^{(1)})(1 - \omega_0^{(\Sigma)}) = 1 - \omega_0 + (1 - \omega_0^{(1)})f^{(1)} \quad (88)$$

Using Eqs. 85, 86, and 88 we can rewrite the forward problem Eqs.6–8, so that atmospheric parameters describing the unknown constituent, $f^{(1)}(\tau)$ and $p^{(1)}(\tau, u)$, enter its operator L and right-hand term S explicitly. In our case of the unknown gas component, $\omega_0^{(1)} \equiv 0$, and Eqs.86, 88 take the form:

$$(1 + f^{(1)})p^{(\Sigma)} = p, \quad (89)$$

$$(1 + f^{(1)})(1 - \omega_0^{(\Sigma)}) = 1 - \omega_0 + f^{(1)}. \quad (90)$$

Obviously, $f^{(1)}$ enters only Eq.6 of the forward problem. Rewriting it in the differential form and using the parameters of the composite atmosphere we have:

$$u dI + I d\tau^{(\Sigma)} - \frac{d\tau^{(\Sigma)}}{2} \int_{-1}^1 p^{(\Sigma)} I du' = (1 - \omega_0^{(\Sigma)}) B d\tau^{(\Sigma)}. \quad (91)$$

Substituting the expression for the optical depth, Eq.85, using Eqs.86, 88 and returning back to the form of differential equation, we obtain the equation of radiative transfer which contains $f^{(1)}$ explicitly:

$$u \frac{dI}{d\tau} + (1 + f^{(1)}) I - \frac{1}{2} \int_{-1}^1 p I du' = (1 - \omega_0 + f^{(1)}) B. \quad (92)$$

Now we can consider the expression for the variation δJ , Eq.22. For variations in the right side of it we have:

$$\delta S = B \delta f^{(1)}, \quad (93)$$

$$\delta LI = I \delta f^{(1)}, \quad (94)$$

Substituting Eqs.93, 94 into Eq.22 and writing the scalar product in it explicitly we obtain after some rearrangements:

$$\delta J(\mu) = \int_0^{\tau_0} d\tau \delta f^{(1)}(\tau) \int_{-1}^1 du (B(T(\tau)) - I(\tau, u)) I^*(\tau, u), \quad (95)$$

from which, comparing with Eq.1, we obtain the expression for the optical mixing ratio weighing functions in the form:

$$\frac{\delta J(\mu)}{\delta f^{(1)}(\tau)} = \int_{-1}^1 (B(T(\tau)) - I(\tau, u)) I^*(\tau, u) du. \quad (96)$$

To convert this expression to that for the gas mixing ratio weighing functions we observe that for the unknown gas constituent, the definition of the optical mixing ratio, Eq.84, can be rewritten in the form:

$$f^{(1)} = \frac{\kappa}{\alpha}, \quad (97)$$

where κ is the absorption coefficient of the unknown gas and α is the extinction coefficient of the background atmosphere. Expressing the gas absorption coefficient, κ through the molecular absorption cross-section, σ , number density of the gas background atmosphere, n_0 , and mixing ratio, f , of the molecules of unknown gas we have:

$$f^{(1)} = \frac{\sigma n_0}{\alpha} f. \quad (98)$$

Thus, if only f is varied, then $\delta \ln f^{(1)} \equiv \delta \ln f$ and we have the following chain of equalities:

$$\frac{\delta}{\delta \ln f} \equiv \frac{\delta}{\delta \ln f^{(1)}} = f^{(1)} \frac{\delta}{\delta f^{(1)}}. \quad (99)$$

Using Eq.98, we obtain:

$$\frac{\delta}{\delta \ln f} = \frac{\kappa}{\alpha} \frac{\delta}{\delta f^{(1)}}. \quad (100)$$

Finally, applying Eq.29 to Eq.26 we obtain the sought expression for the gas mixing ratio weighing functions:

$$\frac{\delta J(\mu)}{\delta \ln f(\tau)} = \frac{\kappa(\tau)}{\alpha(\tau)} \int_{-1}^1 (B(T(\tau)) - I(\tau, u)) I^*(\tau, u) du. \quad (101)$$

To demonstrate that the case of pure absorption, Eq.5 is indeed a particular case of Eq.101 we need the solutions of the adjoint problem for the case of pure absorption, Eq.6, and of its forward counterpart for this case. The form of the forward problem of radiative transfer for this case can be obtained directly from Eqs.2.1–3 letting $\omega_0 = 0$:

$$u \frac{dI}{d\tau} + I(\tau, u) = B(T(\tau)), \quad (102)$$

$$I(0, u) = 0, \quad u > 0, \quad (103)$$

$$I(\tau_0, u) = B_0, \quad u < 0. \quad (104)$$

Its solution for the upwelling radiation, $u < 0$, is:

$$I(\tau, u) = \exp(\tau/\mu) \times \left(B_0 \exp(-\tau_0/\mu) + \frac{1}{\mu} \int_{\tau}^{\tau_0} B(\tau') \exp(-\tau'/\mu) d\tau' \right) \delta(u + \mu) \quad (105)$$

Using integration by parts, applying the definition of transmittance, Eq.78 and assuming $B_0 = B(T(\tau_0))$ we can rewrite Eq.105 in the form:

$$I(\tau, u) = \left(B(T(\tau)) + t(\tau, \mu) \int_{\tau}^{\tau_0} t(\tau', \mu) dB(T(\tau')) \right) \delta(u + \mu). \quad (106)$$

Substituting expressions for I^* , Eq.76, and for I , Eq.105, into Eq.30 we have:

$$\frac{\delta J(\mu)}{\delta \ln f(\tau)} = -\frac{1}{\mu} \cdot \frac{\kappa(\tau)}{\alpha(\tau)} \int_{\tau}^{\tau_0} t(\tau', u) dB(T(\tau')). \quad (107)$$

Finally, changing from the vertical coordinate τ , $d\tau = \alpha dz$, to $\ln p$, $d \ln p = dz/H_g$, we have to multiply Eq.107 by factor

$$d\tau/d \ln p = \alpha H_g. \quad (108)$$

We then obtain the expression for pure absorption in the form of Eq.5.

5 Discussion and conclusion

We considered the operator formulation of the adjoint approach to the sensitivity analysis and applied it to the problem of evaluation of temperature and mixing ratio weighting functions for remote sensing of plane-parallel scattering atmospheres in thermal IR. The analytic expressions for these weighting functions were obtained that contain the solution of the adjoint problem of radiative transfer $I^*(\tau, u)$, and, in the case of the mixing ratio weighting functions, also the solution of the conventional, forward problem of radiative transfer. It was demonstrated that obtained expressions converge to known expressions for the case of pure absorption when atmospheric scattering can be neglected.

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